



2011 DOE Office of Vehicle Technologies Program Review

Low Temperature Automotive Diesel Combustion

Light-Duty Combustion Experiments

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Light-Duty Combustion Modeling

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Project ID# ACE002



Overview

Timeline:

- Project has supported DOE/industry advanced engine development projects since 1997
- Direction and continuation evaluated yearly

Budget:

DOE funded on a year-by-year basis

- SNL \$730k (FY11), \$725k (FY10)
- UW \$230k (FY11), \$230k (FY10)

Barriers addressed:

- A Lack of fundamental knowledge
- B, G Lack of cost-effective emission control
- C Lack of modeling capability

Technical targets addressed:

- 40% diesel fuel economy improvement
- Tier 2, bin 2 emissions
- Emission control efficiency penalty < 1%
- 30 \$/kW power specific cost

Barriers/T argets from EERE-VT 2011-15 Multi-year program plan)

Partners:

- 20 industry/national laboratory partners in the Advanced Engine Combustion MOU
- Close collaboration with GM-funded research at UW (Foster)
- Additional post-doc funded by GM



Relevance of Sandia's major technical accomplishments (May 2010 – March 2011)

- 1 Varied ignition quality and volatility independently in an orthogonal matrix to examine the impact of these fuel properties on LTC CO and UHC emissions**
Barriers/Targets: Improved fundamental understanding of the role of fuel properties on enabling LTC combustion; fuel property parameter sweeps for modeling validation & sensitivity studies; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement ([links to UW 1](#))
- 2 Assessed accuracy and implementation of RNG turbulence models**
Barriers/Targets: Improved modeling of in-cylinder processes ([UW 2](#))
- 3 Examined asymmetries and mean flow structure in the induction flow via Particle Image Velocimetry**
Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes ([UW 3](#))
- 4 Investigated wall-wetting by post-injections for PM trap regeneration for various injection timings and diesel/biodiesel fuel blends**
Barriers/Targets: Improved understanding of in-cylinder processes (penetration, spray disruption by exhaust flows); efficiency penalty of PM trap regeneration; 30 \$/kW cost target
- 5 Consolidated measurements and simulations to provide a phenomenological picture of light-load LTC combustion**
Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement ([links to past UW work](#))

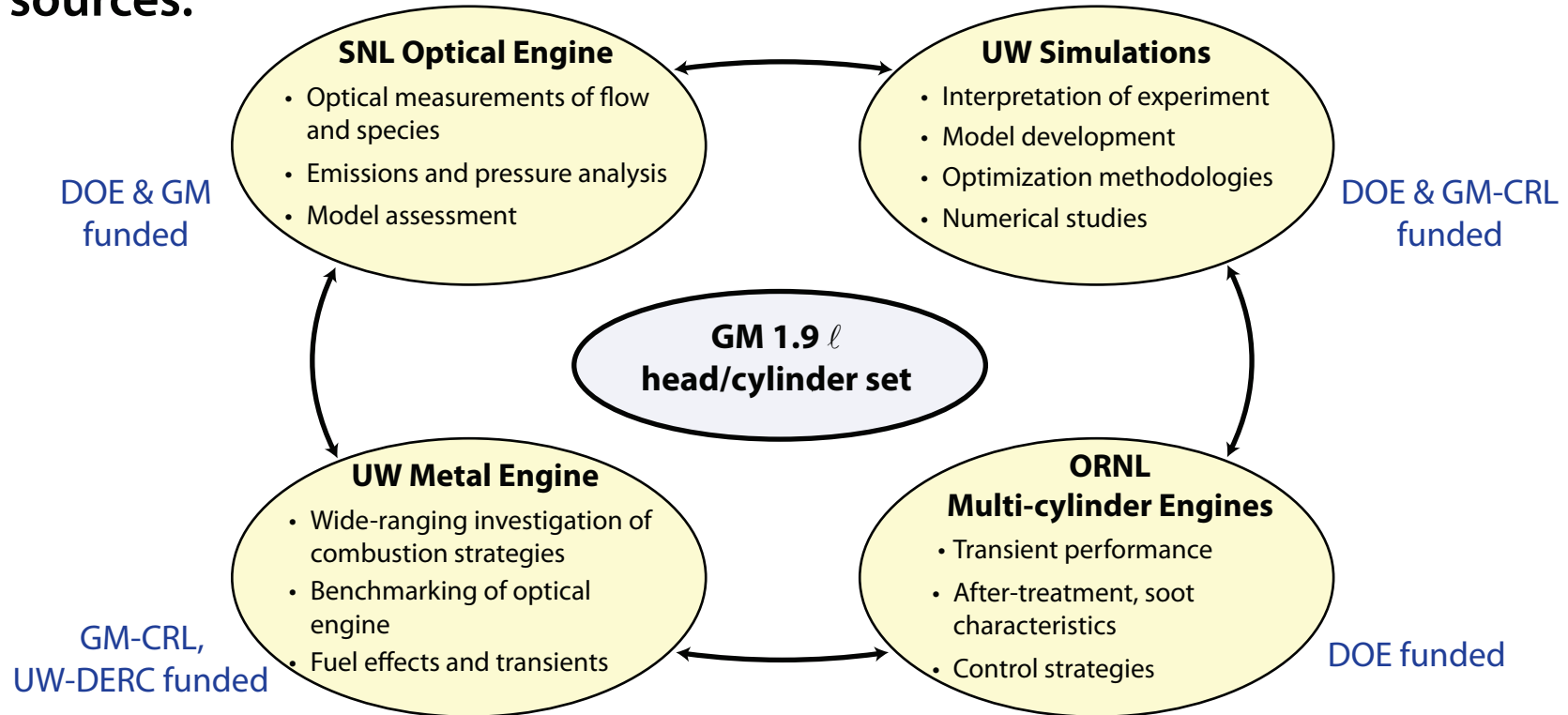


Relevance of UW's major technical accomplishments (May 2010 – March 2011)

- 1 Examined sources of discrepancy in UHC and CO distributions between model and experiment & identified spray/entrainment model as a dominant source**
Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement ([links to SNL 1](#))
- 2 Evaluated variable density gas jets and engine flows with RNG turbulence closure; derived alternative model dependent on the 'dimensionality' of the strain**
Barriers/Targets: Improved modeling of in-cylinder processes ([SNL 2](#))
- 3 Examined intake flow modeling with detailed port, valve, and combustion chamber mesh; examine impact of flow-field non-uniformities on UHC and CO**
Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement ([SNL 3](#))
- 4 Examined light-duty RCCI combustion; upgraded engine fuel system(s)**
Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvements
- 5 Improved soot model based on PAH kinetics; compared results to conventional, PCCI, and RCCI combustion in light- and heavy-duty engines**
Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement; cost-effective emission control

Technical/Programmatic Approach

Our approach coordinates and leverages the strengths of several institutions and funding sources:



Programmatic:

- Multi-institution effort focused on a single hardware platform
- Significant leverage of DOE funds by support from other sources

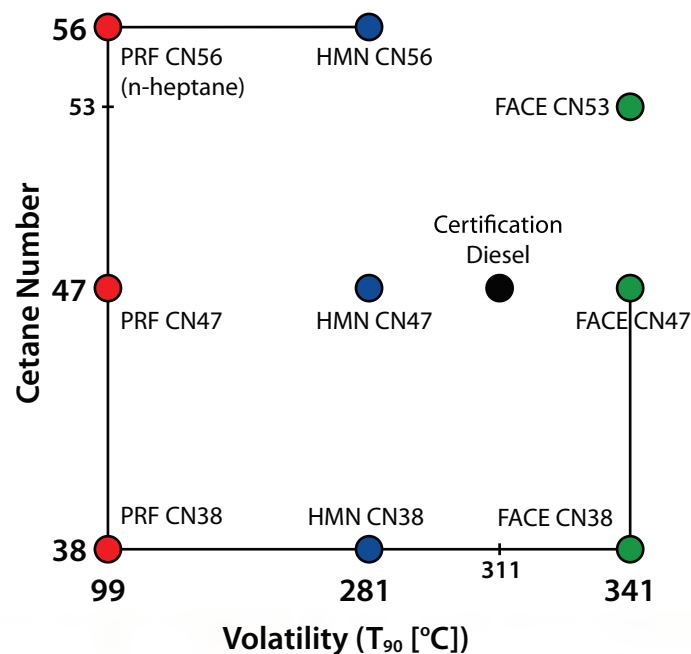
Technical:

- Closely coordinated program with both modeling and experiments
- Input from and technical transfer to industry inherent in program structure

Accomplishments: In-cylinder sources of UHC/CO

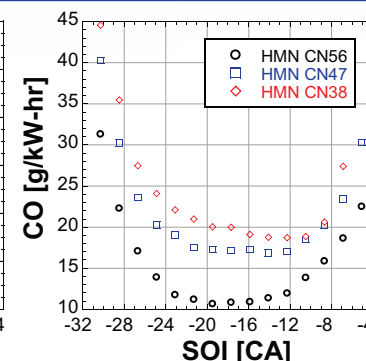
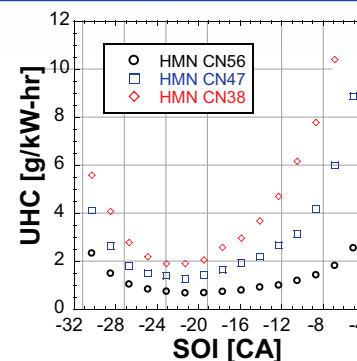
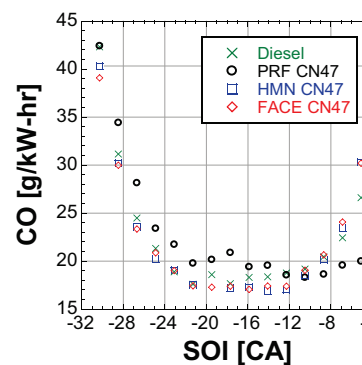
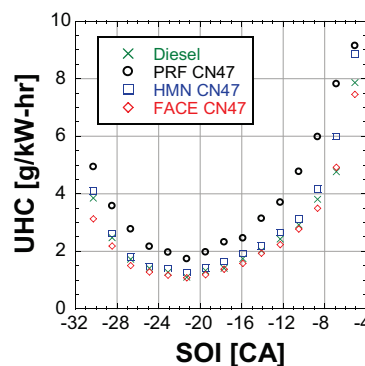
Task:

Investigate the impact of fuel ignition quality and volatility on the UHC/CO emissions and combustion efficiency of PCI LTC through measurements made in an orthogonal fuel property matrix



Results:

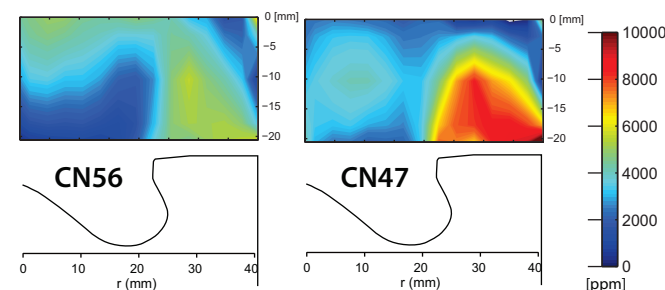
Cetane number is the dominant fuel property impacting UHC & CO



Large volatility changes are needed to impact engine emissions

Images show that despite greater piston films and crevice UHC, low volatility fuels provide lower bulk gas UHC & CO

High ignition quality likewise lowers bulk gas UHC & CO

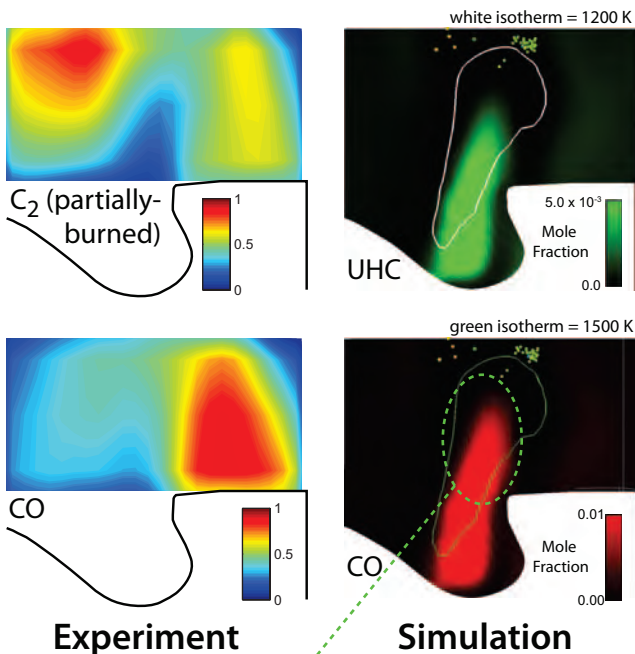


Variation in bulk gas CO as cetane number varies with fixed volatility (UHC is similar)

Accomplishments: In-cylinder sources of UHC/CO

Task:

Identify the source of the discrepancy between the experiments and regarding the dominant in-cylinder source of UHC and CO emissions



Undermixed plume leaving the bowl is not seen experimentally

Results:

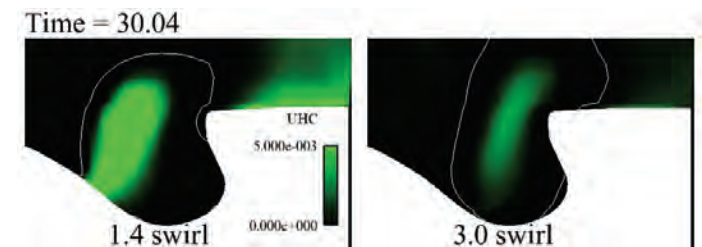
Previous work demonstrated that:

- Improvements to reduced kinetic mechanism helped, but did not fully resolve the discrepancy
- Investigated sensitivity to T_{in} , grid resolution, O_2 , bowl volume, C_d
- Remaining discrepancy associated with mixing processes

This year have investigated model sensitivity to:

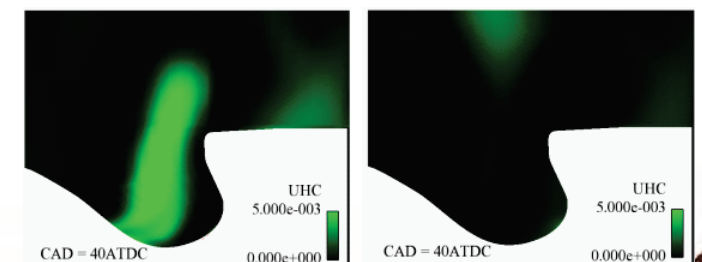
- R_s , "swipro", P_{inj} , T_{wall} , SOI, m_{fuel} , turb. & wall impingement models

Results have the greatest sensitivity to R_s and P_{inj}



But the most promising improvement was associated with the new gas jet spray modeling:

Future work will focus on model tuning to predict a range of R_s , P_{inj} , and d_{nozzle}



Accomplishments: Turbulence model assessment

The flow and turbulence modeling underpins the simulation of the mixing and combustion processes

Background:

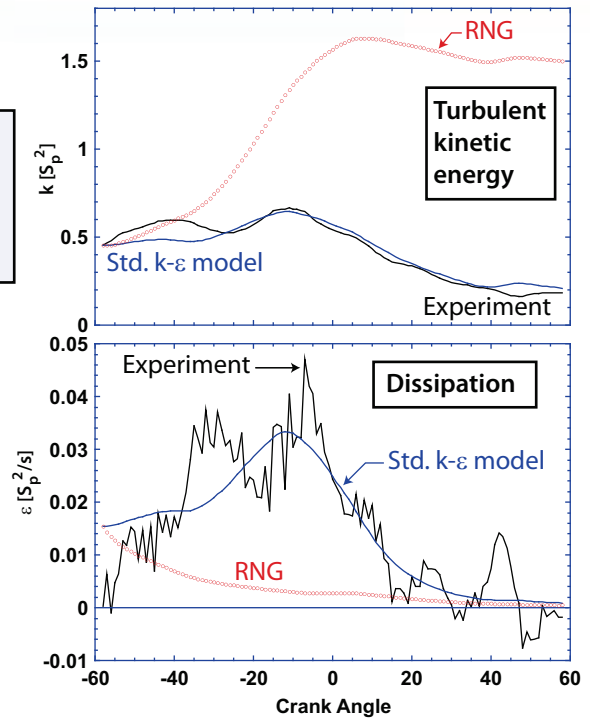
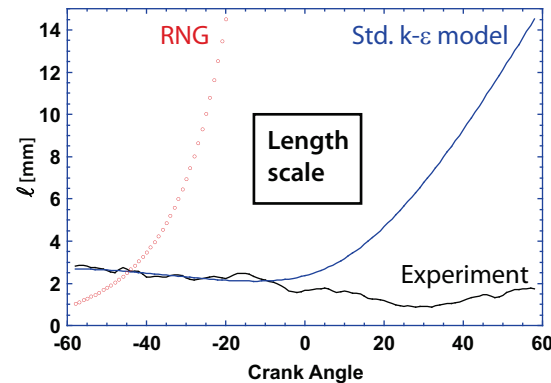
Standard k - ε turbulence modeling cannot predict both compression and expansion with a single set of constants

Task:

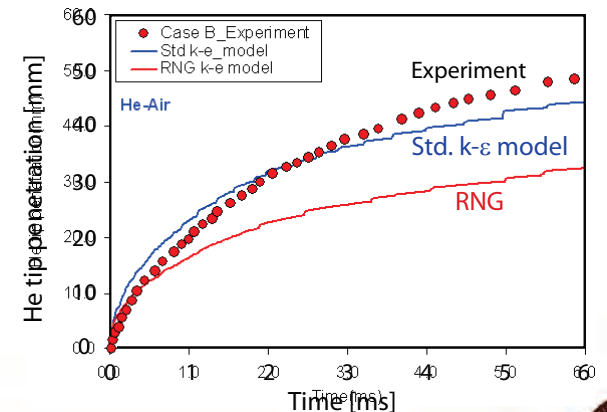
Investigate the performance of the (variable constant) RNG k - ε model

Results:

The RNG closure severely overestimates k and ℓ , due to the underestimation of ε



The penetration of variable density gas jets is under-predicted for the same reasons



Accomplishments: Turbulence model shortcomings: causes and redress

KIVA RNG k - ε coding:

```
if(diverg(i4).gt.0.0) then
  ce3=0.41333+0.06899*reta*retaeq
else
  ce3=0.41333-0.06899*reta*retaeq
endif
```

$$C_3 = \frac{-4+2C_1}{3} + \frac{1}{(\nabla \cdot \mathbf{U})} \frac{1}{v} \frac{dv}{dt}$$

$$+ \frac{\sqrt{6}}{3} C_\mu \frac{\eta^2(1-\eta/\eta_0)}{1+\beta\eta^3} (-1)^\delta$$

$$\eta = \left(\frac{k}{\varepsilon} \right) \sqrt{2 S_{ij} S_{ij}}$$

As implemented, C_3 is computed as strain rate (S_{ij}) dependent – it is not evaluated in the rapid distortion limit

In this case, the RNG-specific terms are:

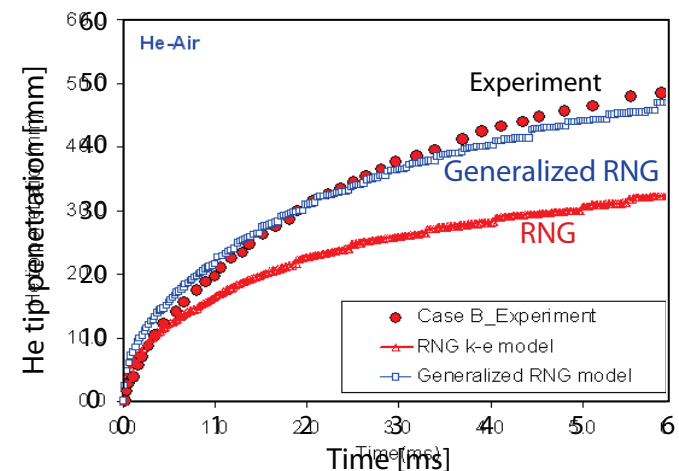
$$\mathcal{R} + C_{3,\eta} \varepsilon (\nabla \cdot \mathbf{U}) = \frac{C_\mu \eta^2 (1 - \eta/\eta_0) \varepsilon}{1 + \beta \eta^3} \left[\underbrace{\sqrt{2 S_{ij} S_{ij}} - \frac{\sqrt{6}}{3} |\nabla \cdot \mathbf{U}|}_{\text{Difference between the characteristic strain rate and the characteristic rate associated with pure spherical distortion, } S_{11} = S_{22} = S_{33} = (\nabla \cdot \mathbf{U})/3} \right]$$

Difference between the characteristic strain rate and the characteristic rate associated with pure spherical distortion, $S_{11} = S_{22} = S_{33} = (\nabla \cdot \mathbf{U})/3$

In this implementation, the model behaves considerably better (similar to k - ε), though it has no physical/mathematical basis

Redress:

An alternative compressible RNG closure based on the 'dimensionality' of the flow field has been developed and is being tested



Future work will focus on more thorough model testing against engine measurements and DNS calculations

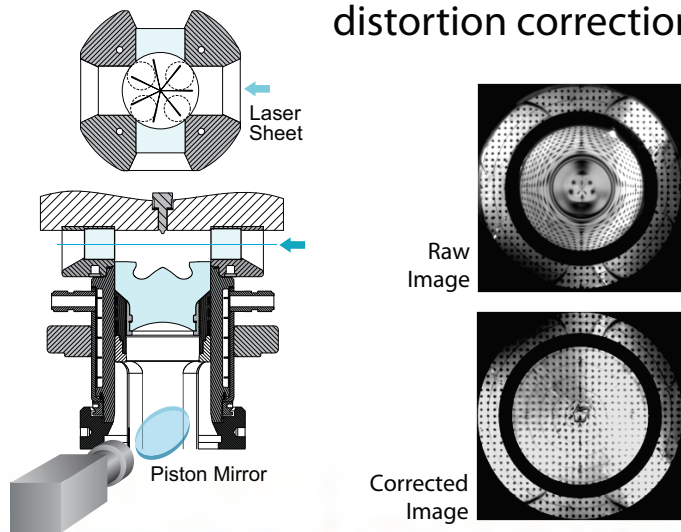
Accomplishments: In-cylinder flow characterization

Task:

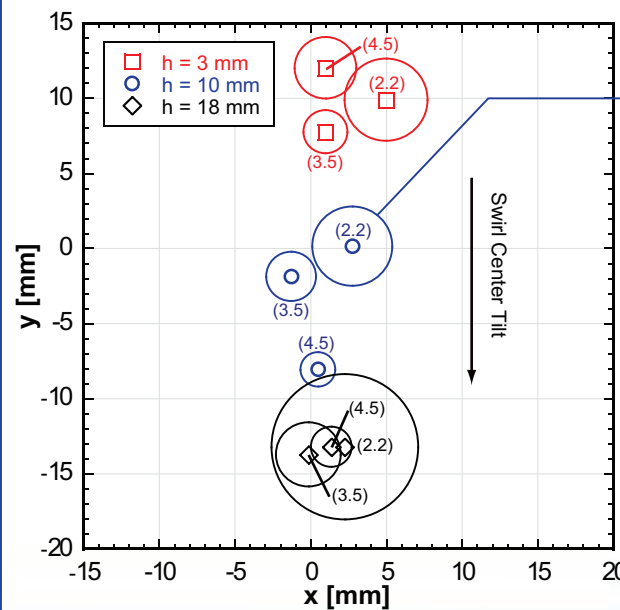
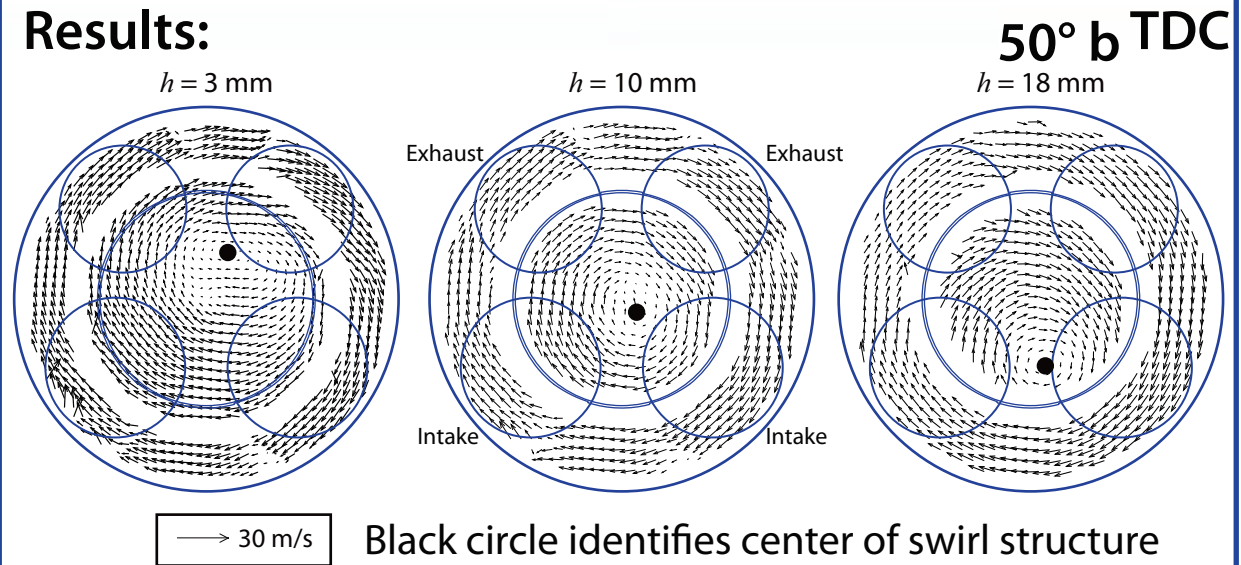
Characterize in-cylinder flow structure to:

- Validate induction stroke calculations
- Clarify flow structure for closed-cycle simulations
- Evaluate asymmetry of the pre-combustion flow (need for 360° grid)

Method: Horizontal Plane PIV with distortion correction



Results:



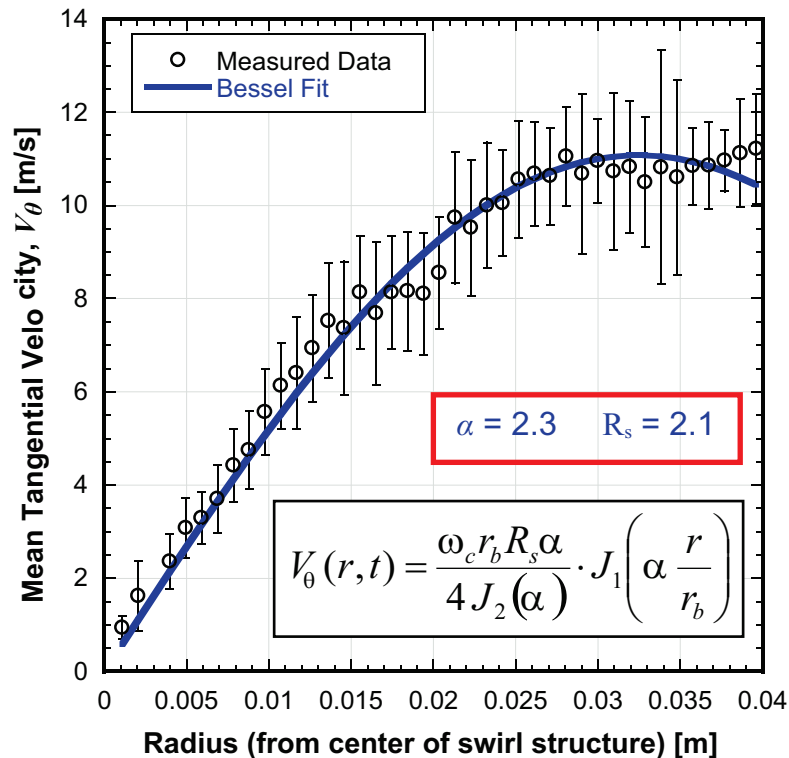
Numbers in parenthesis represent swirl ratio, circles represent 1- σ deviation

Swirl center tilt (and pre-cessional motion) is:

- Insensitive to swirl ratio
- Present in individual cycles
- Less variable at high R_s

Accomplishments: In-cylinder flow characterization

Results:



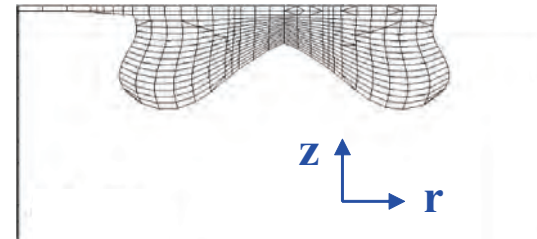
The average value of α ("swipro") over all swirl ratios and measurement locations is

$$\alpha = 2.2$$

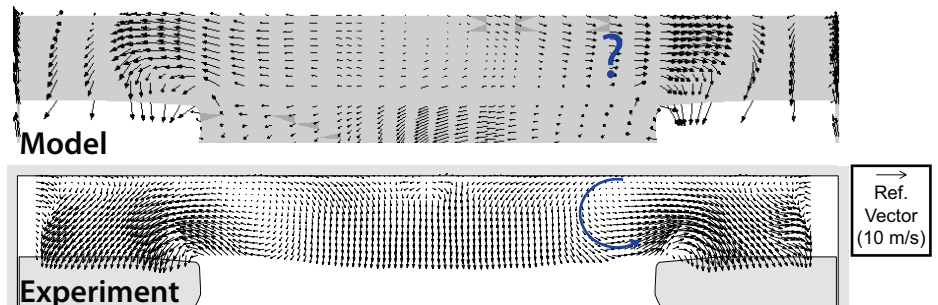
Comparison with previous LDV data suggests this value is independent of port geometry

Comparison with model results:

A full 3-d mesh of the GM engine has been created



Comparison with horizontal and vertical plane PIV measurements, for various turbulence models, is in progress (Note the absence of a major clearance volume vortex)



Accomplishments:

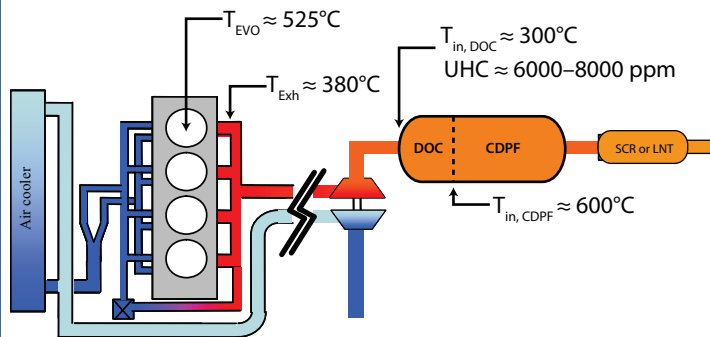
Post-injection wall wetting with biofuel blends

Task:

Examine the impact of biodiesel content on wall-wetting when post-injections for DPF regeneration are employed

- i) Neat D2 versus biofuel blends
- ii) Impact of injection timing
- iii) Potential for jet disruption by exhaust flows

Method:



Simulate in cylinder conditions typical of highway-like PDF regeneration (5 bar, 1500 rpm) assuming a close coupled DOC

Results:

With early post-injection, none of the fuels wet the cylinder wall (consistent with liner friction studies)

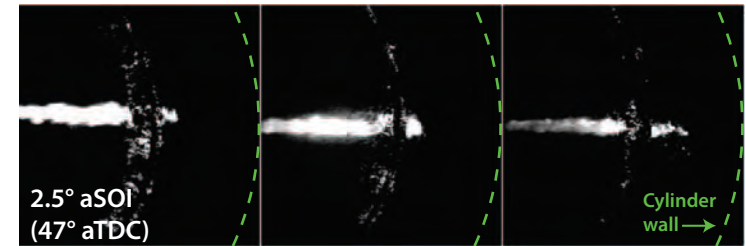
All of the fuels impact the cylinder wall with conventional timing, even with small post-injection quantities
Wetting is more severe and persistent with biofuel blends

Injection during the exhaust blowdown period fails to significantly disrupt jet penetration

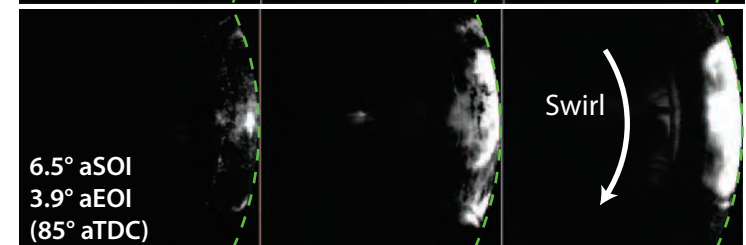
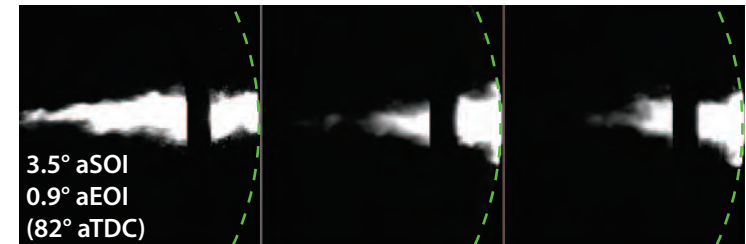
Cert. D2

PME20

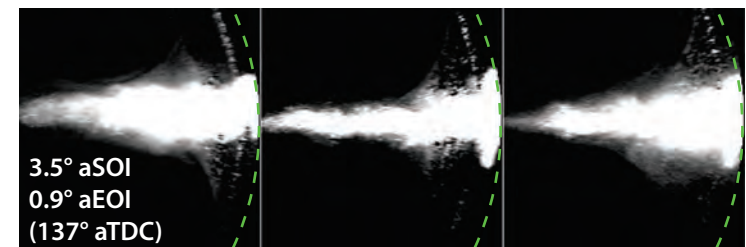
SME100



SOI=44.5° aTDC, m=5.1 mg, P=20 bar, T=1100 K



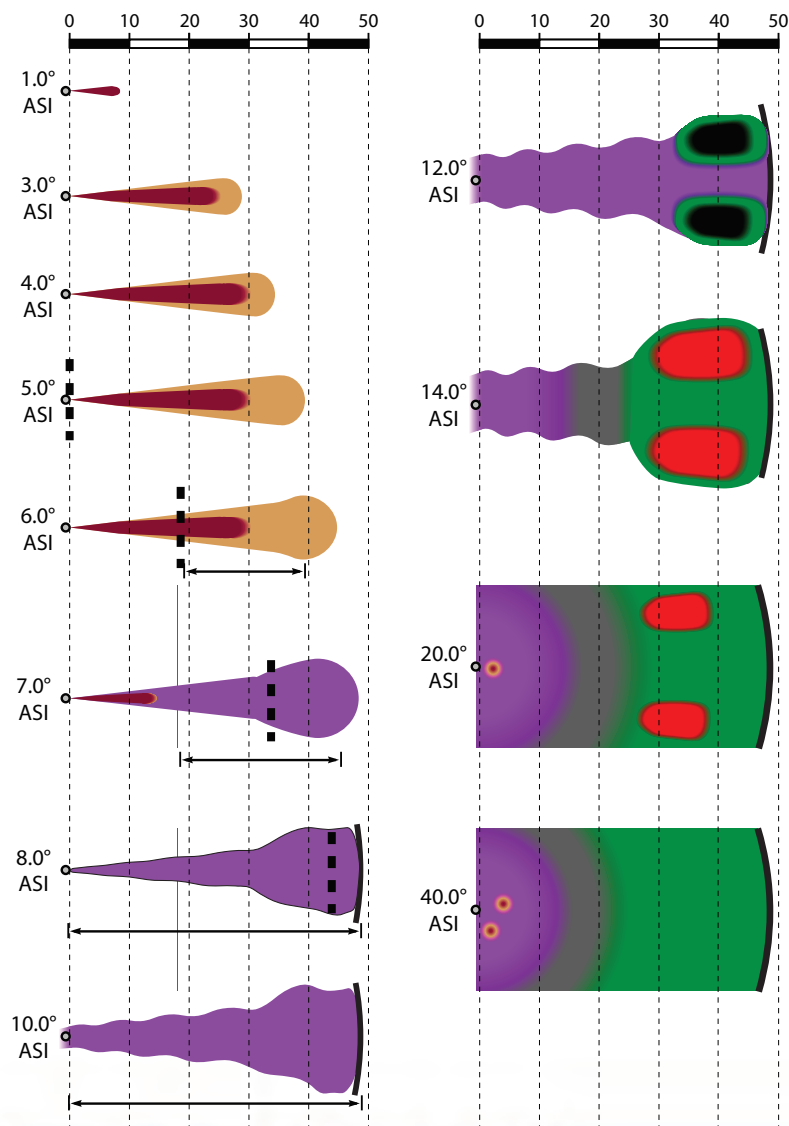
SOI=78.5° aTDC, m=3.3 mg, P=7 bar, T=900 K



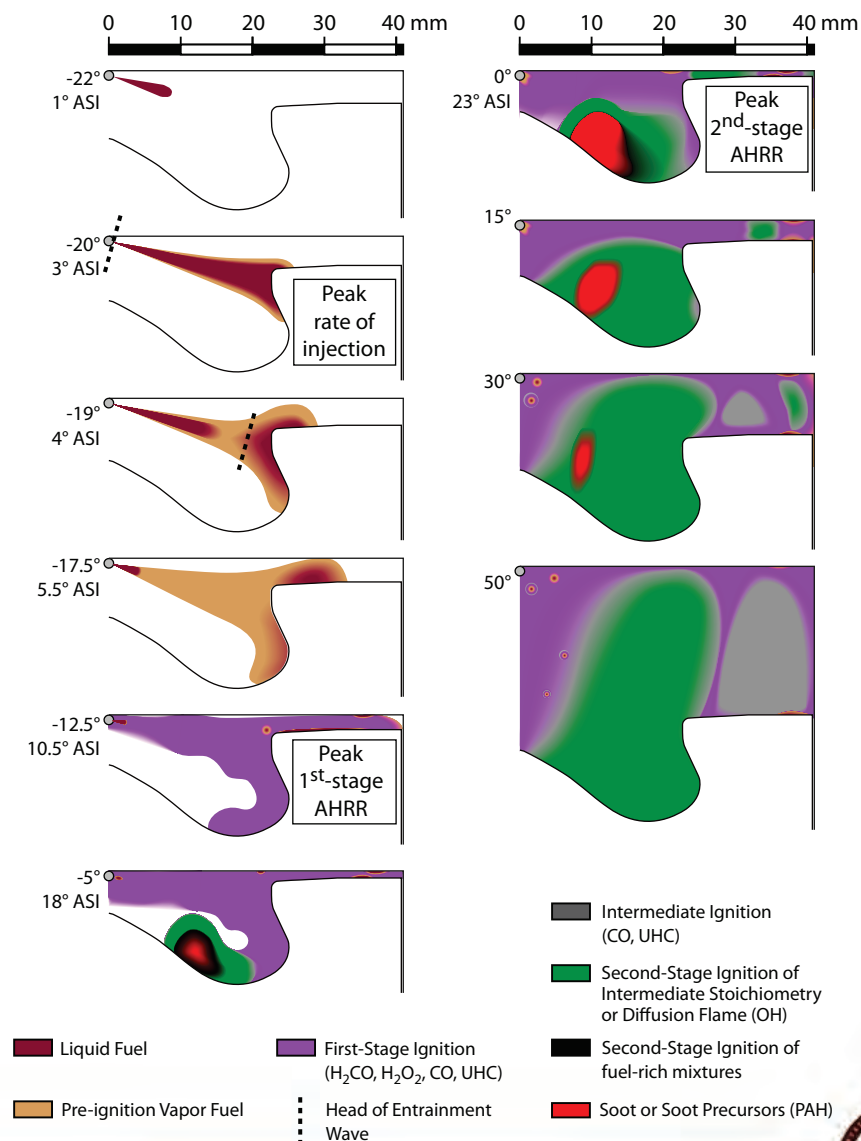
SOI=133.5° aTDC, m=3.3 mg, P=3.5 bar, T=750 K

Accomplishments: Data consolidation and phenomenological picture of light-duty LTC

Heavy-duty LTC (Musculus & Pickett)



Light-duty, early-injection LTC



Collaborations

Within Vehicle Technologies program:

- Formal collaboration between SNL-UW-ORNL
- Participation in Advanced Engine Combustion group, including presentations and discussion with 20 industrial/national laboratory partners:



Ex-Vehicle Technologies program:

- Close ties with GM:
 - GM-funded post-doctoral researcher
 - Monthly teleconferences (Diesel and LES working groups)
- Strong ties to Lund University:
 - Exchange students perform research at Sandia
 - SNL staff participates in LU research projects

Future work – SNL/UW

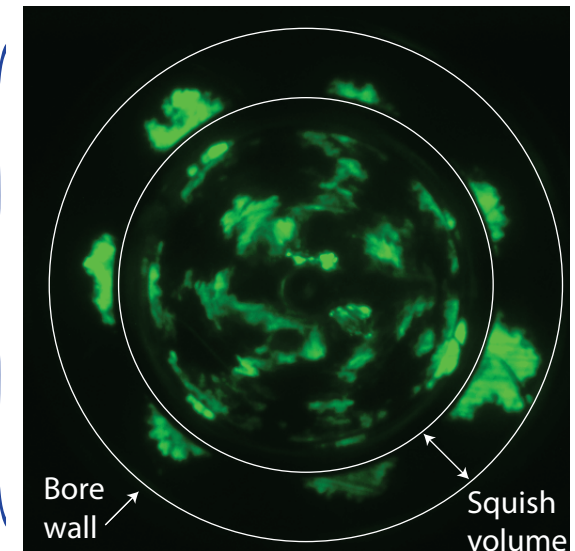
- Examine the impact of various engine design and operating parameters on in-cylinder sources of UHC and CO:
 - Swirl ratio, injection pressure, hole size
 - Multiple injections

Demonstrate/develop a predictive modeling capability

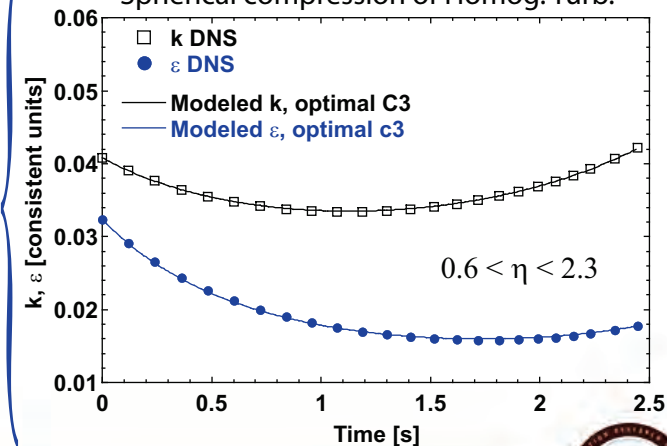
- Measure pre-combustion equivalence ratio distributions to aid in model validation and interpretation of UHC/CO data
- Continue work on validating or developing new RANS-based turbulence models to enable more accurate dissipation modeling (compare to existing / new high-Re DNS calculations – Joe Oefelein)
- Investigate the impact of flow and geometric asymmetries on combustion and emission formation (Extend PIV measurements to squish volume near TDC, horizontal plane UHC imaging near TDC)

Demonstrate develop capability to quantitatively predict flow structures, including asymmetries

Fuel fluorescence measured 15° bTDC



Comparison with low Re DNS (Wu, 1985)
Spherical compression of Homog. Turb.





Summary

- **Project focuses on several barriers/targets identified in the EERE-VT program plan:**
 - Lack of fundamental knowledge
 - Lack of modeling capability
 - 30\$/kW specific cost; Tier 2, Bin 2 emissions
 - Lack of cost effective emission controls
 - Emission control efficiency penalty
 - 40% diesel fuel economy improvement
- **Technical accomplishments this reporting period include:**
 - Understanding of the impact of fuel properties on LTC UHC/CO in-cylinder emission sources
 - Improved modeling of LTC combustion and UHC/CO emissions
 - Identification of problems with compressible RNG turbulence model and implementations
 - New compressible RNG closure model dependent on mean flow 'dimensionality'
 - Measurement of swirl flow structure and asymmetries; full 360° grid and initial simulations
 - Imaging study of post-injections spray wall impingement for neat diesel and biofuels
 - Consolidation of data and development of phenomenological picture of light-duty LTC to complement heavy-duty work
- **Future work will include:**
 - Continuation of UHC/CO imaging and modeling, with emphasis on capturing the influence of engine design and operating parameter dependence; measurement of pre-combustion ϕ -dist.
 - Continued efforts to improve compressible RANS flow modeling – which underpins the modeling
 - Continuation of flow (and horizontal plane UHC distributions), with an emphasis on understanding asymmetries and the necessity of modeling them